



Renewable chemical feedstock supply network design: The case of terpenes

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ABSTRACT

Designing supply networks enabled by renewable chemical feedstocks presents complexities in terms of undefined markets, multiple intermediate chemical compound options and uncertain chemical conversion pathways. This research addresses this gap by developing a structured approach for designing compound class defined supply chains (SCs) through involving the analysis of: (i) renewable chemical feedstock sources; (ii) alternative technology and processing options; (iii) intermediate or end-user markets; and (iv) commercial value and viability. In particular, we apply this approach on the promising case of terpenoid feedstocks. Further, in the specific case of terpenes we analyse renewable feedstock SC options for the production of 'green' pharmaceuticals demonstrated by a case study on paracetamol. To that end, evidence is obtained through collating the dispersed literature on renewable chemical feedstocks, by semi-structured interviews and through expert panel engagements involving industry and academic informants. The study findings inform about the systemic mapping and modelling of compound class defined material-processing-supply networks, further providing a basis to identify feasible intermediate and final product options. The research contributes to the operations management academic and practice literature by proposing a structured approach for mapping and designing renewable chemical feedstock SCs from a source material perspective, in this case renewable terpenoid feedstocks, in contrast to the traditional end-market applications. From a circular economy perspective, the use of renewable feedstocks in extended SCs demonstrates the utility of the approach by integrating supply side considerations (i.e. feedstock) with uncertainties of intermediate processing options and commercialisation routes.

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1. Introduction

The chemical industry is recognised as a frontrunner in sustainable supply chain (SC) practises (Padhi et al., 2018), owing to its primary reliance upon petroleum-based chemical feedstocks (Keim, 2010). Indicatively, the chemical sector has been growing considerably during the recent decades with a global value of US\$ 171 billion in the 1970's to US\$ 4,120 billion in 2012 (UNEP, 2013). Therefore, the associated detrimental environmental repercussions are motivating policy-makers and industry stakeholders to investigate novel ways to continuously improve sustainability across chemical value chains (Iles and Martin, 2013). The industry's

growth and environmental impact is clearly illustrated by two representative examples. Firstly, the total chemical fiber output in China, the largest producing country in the world, increased from around 23% in 2002 to almost 70% in 2012, with a projected average annual growth rate of 15% due to the increasing global demand for chemical fiber products (Lin and Zhao, 2015). Secondly, in 2013 the chemical enterprises in the United States of America were responsible for approximately 42% of the total volume of industrial hazardous wastes (Cespi et al., 2016). In this sense, integrating the notion of circular economy in chemical industrial systems can ensure the sustainability and long-term viability of the sector (Genovese et al., 2017).

The circular economy discourse exerts pressure on the frontiers of sustainable SC management by emphasising the idea of value creation and viability assurance in production and consumption systems. In particular, it focusses on mitigating resources'

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appropriation and valorising waste streams (Srai et al., 2018). In this regard, circular business models (Geissdoerfer et al., 2018) and sustainable manufacturing practices (Moktadir et al., 2018), along with workable relationships in the triplet ecology-economy-society (Genovese et al., 2017), are considered from an end-to-end SC perspective. To facilitate the transition from linear supply systems to equivalent circular SCs, a variety of nascent conceptual frameworks has been presented in the extant literature (Korhonen et al., 2018). However, existing research studies lack formalisation of circular SC design strategies and principles that could be directly applied in real-world industrial cases (Prieto-Sandoval et al., 2018), such as in the chemical industry.

The exploitation of renewable materials as substitutes to petroleum-based feedstocks has great potential (Hennig et al., 2016), with a vast array of value-added applications including chemicals, pharmaceuticals and electronics (Kawaguchi et al., 2016). In particular, terpenes, a large and diversified class of hydrocarbons, are recognised by academics and industry actors as novel sources of renewable chemical feedstocks that could be used as value-added substitutes to petrochemical equivalents in upstream supply network operations (Behr and Johnen, 2009). For example, Wu and Davis (2016) reported the experimental conversion of algae biomass into terpenes for the production of high energy density aviation fuels, while Nuutinen (2018) reviewed the evidenced pharmacological potential of terpenes found in cannabis and hops.

Nonetheless, adopting a circular view in chemical SCs defined by renewable chemical feedstocks requires that a range of critical factors are explored (Sheppard et al., 2011), including: availability of sustainable feedstock sources; technical feasibility of feedstock processing options; distribution requirements; and market opportunities. The European Bioeconomy Panel documented that the aforementioned issues had not been sufficiently addressed (European Bioeconomy Panel, 2014), hence hindering the implementation of the European Bioeconomy Strategy and Action Plan (COM(2012) 60 final) (Commission Communication COM, 2012). Furthermore, owing to the plethora and structural diversity of available renewable feedstocks, like terpenes with over 55,000 structurally similar compounds (Wu and Davis, 2016), the need for mapping techniques and network configurations that promote the understanding of SCs arising from alternative renewable chemical feedstocks is evident for both academics and industrial stakeholders alike. The key identified academic and industrial challenge is thus to design circular value chains involving renewable compounds.

From an academic point of view, literature on the design of circular SCs defined by renewable chemical feedstocks is scant (Tsolakis et al., 2016), yet possess an interesting field for research advocacy bodies (Ellen MacArthur Foundation, 2015). Indicatively, in the United Kingdom, the Engineering and Physical Sciences Research Council (EPSRC) recently awarded, through its sustainable chemical feedstocks' panel, a total of six research grants focusing on renewable chemical compounds with a total budget of over £ 12 million (Tsolakis et al., 2016). A categorisation of extant research and business studies on SC management nonetheless reveals that supply networks are generally analysed from a technology, product, firm and/or market level (Tsolakis et al., 2016). Therefore, an apparent research gap exists in the structured analysis of compound class defined supply networks. Recently, Tsolakis and Srai (2018) provided a System Dynamics-based mapping methodology for capturing the macro-level supply network interrelations and causal effects in industrial systems that exploit renewable chemical feedstocks. Furthermore, Srai et al. (2018) provided a decision-making framework for investigating viable configuration opportunities for SCs arising from renewable chemical feedstocks.

Nevertheless, existing studies have a generic view over renewable materials without focusing on a specific class of intermediate compounds like terpenes.

From a corporate perspective, the interest with regards to applied circular economy business models and manufacturing operations is substantial. Veleva and Bodkin (2018) reported the growing number of partnerships between well-established companies and entrepreneurs to advance circular economy principles within their manufacturing networks. BASF, the largest chemical company in the world with US\$ 56.86 billion in revenues (Statista, 2018), exploits the use of renewable feedstocks for the manufacturing of selected intermediate and final products owing to (BASF, 2018): (i) the interest of consumers and retailers for such offerings; and (ii) the development of functional molecules not feasible through fossil-based synthesis pathways. Nonetheless, a structured approach for the identification of attractive value propositions that emerge from the potential intermediate compound, derived from a given feedstock, is lacking. Such systemic mapping and modelling approaches of compound class defined material-processing-supply networks could inform and guide companies on the design and analysis of respective circular value chain operations.

This research focuses on the analysis and design of circular supply networks defined by renewable feedstocks, particularly focusing on terpenes which are compounds available in plant-based biomass and industrial waste streams. The case of terpenes is selected as the object of analysis in this research by virtue of: (i) the prolific biogenic production of terpenes amounting to 10^9 tonnes per year at a global scale (Hocking, 2006); (ii) the promising industrial-scale production of terpenes, via low-cost processing of plant sugars and cellulosic waste, which is projected at a scale of millions of tonnes per year (Leavell et al., 2016); (iii) the flexible supplies of naturally occurring and/or engineered terpenoid feedstocks (Mewalal et al., 2017); and (iv) the compatibility of terpenes to existing petroleum-based processing routes and installed manufacturing technologies due to their hydrocarbon structure (EPSRC, 2012). Ding and Matharu (2014) further suggested that terpenes should not be investigated myopically but, to ensure sustainability gains, must be considered holistically from an end-to-end SC viewpoint. Terpenes have the potential to complement carbohydrate, oil and lignin-based feedstocks as replacements for petrochemicals in a wide range of commercial products like flavours and fragrances, pine oils, insecticides, pharmaceuticals and fuels (Silvestre and Gandini, 2008). However, current research on terpenes is mainly limited to experimental evidence demonstrating the technical feasibility of compounds in manufacturing operations. Systematic value chain mapping and modelling techniques that encompass a series of renewable terpenoid feedstocks, feasible chemical conversion pathways, viable market options and value delivery platforms are lacking. To that end, a network mapping approach that could guide the design and analysis of terpene-based circular SCs could embrace the four interconnected and mutually interacting theme areas proposed by Srai et al. (2018), namely: (i) renewable chemical feedstock; (ii) technology; (iii) market; and (v) value and viability. This analysis methodology can inform the integrated assessment of renewable feedstock sources, manufacturing technologies and resulting value-added intermediates or end-products in a concise manner. Moreover, considering the complexity associated with the adoption of renewable compounds, uncertainty dimensions and causes thereof have to be analysed for the viability assessment of terpenes.

Overall, the commercial potential of terpene-based monomers and polymers is sufficiently justified in the extant body of literature (Kleij, 2018). However, research on terpene-based manufacturing value chains that identifies a range of feasible intermediates and

final product options is rather myopic. The aim of this research study is to position terpenes within a circular SC context by investigating the design and analysis of alternative network configurations via attempting to answer the following research questions:

- Research Question #1: How should academic and business stakeholders navigate value chain analysis, design and management options defined by terpenes?
- Research Question #2: What is a fundamental network structure that could guide the deployment of supply network operations defined by terpenoid feedstocks?
- Research Question #3: Which are the key uncertainty dimensions that could impact the value and viability of terpene-based circular supply networks?

All the above research queries are critical to be answered since terpene-based SCs appear to comprise a representative paradigm of circular supply networks (Genovese et al., 2017). However, structured approaches for mapping, designing, modelling, and implementing compound class defined material-processing-supply network systems have yet to be demonstrated at an industrial scale. Thus, Research Question #1 calls for the adaptation of traditional end-market oriented SC analysis techniques to enable compound class defined SC designs. Thereafter, the theme areas of analysis for circular SCs defined by renewable chemical feedstocks, in tandem with primary evidence, are leveraged to propose a network structure in order to address Research Question #2. Finally, uncertainties that could undermine the commercial value and viability of terpene-based supply networks are identified to tackle Research Question #3.

This paper follows a multi-method approach to address the enunciated research questions and develop evidence-informed management knowledge in the circular SC management field. The research approach implements a compound class defined SC analysis approach based on the theme areas outlined by Srai et al. (2018), namely: (i) feedstock sources; (ii) technology and processing options; (iii) markets; and (iv) value and viability, to answer Research Question #1. Evidence is obtained through synthesising the dispersed literature on terpenoid feedstocks while semi-structured interviews and expert panel engagements involving academic and industry informants were used to test, refine and validate the outputs necessary to answer Research Question #2. The overall research outcomes provide insights regarding Research Question #3 and demonstrate that the analysis and design of SCs enabled by terpenes lead to radical (re)configuration opportunities with diverse critical uncertainties challenging the commercial viability of relevant network structures. The nature of our approach is recommended in order to provide a robust base for theory building in the circular SC field. Literature evidence (Eisenhardt and Graebner, 2007) along with empirical insights from case studies (Rowley, 2002) assist in theory development. Therefore, we contribute to the academic and practice literature by developing a structured approach for the design of SCs defined by the source material, rather than the traditional end-market application, via: (i) collating the dispersed literature on renewable chemical feedstocks; (ii) conducting semi-structured interviews and expert panel engagements; and (iii) exploiting a real-world case study. From a circular economy perspective, the use of renewable feedstocks in extended SCs demonstrates the utility of the approach by integrating supply side considerations (i.e. feedstock) with uncertainties of intermediate processing options and commercialisation routes.

The remainder of the paper is structured as follows. In Section 2, we provide a description of the materials and methods used to

conduct this study. In Section 3, we explore SC alternative (re) configuration options for the case of terpenes as an illustrative paradigm of renewable chemical feedstocks, based on identified theme areas of analysis. Following that, in Section 4 we provide an integrated structure for circular supply networks defined by terpenoid feedstocks and we further identify the underlying uncertainty dimensions. Section 5 briefly discusses a real-world case of a 'green' pharmaceutical product and the associated SC implications stemming from the utilisation of terpenes. Finally, conclusions, limitations and recommendations for future research beyond the state-of-the-art are discussed in the last Section 6.

2. Materials and methods

2.1. Basic terminology

The circular economy concept can be described based on a plethora of academic or practice-driven definitions (Kirchherr et al., 2017). Despite the divergent understanding of the circular economy concept, existing studies share a similar vision (Prieto-Sandoval et al., 2018): propel the sustainable development of economic systems. With regards to the sustainable SC management field, in this research we adopt the view of Nasir et al. (2017) who identified circular supply networks as value chains in which wasted material flows are exploited as production inputs. Our analysis specifically focuses on the structural configuration and uncertainties governing terpene-based supply networks to make direct inferences to sustainable SC management theory and practise.

Terpenes are a class of naturally occurring chemical compounds with near zero oxygen content, high energy density and diverse biological functionalities (Wu and Davis, 2016); hence, terpenes can be regarded as a sustainable feedstock for the fine chemical synthesis of value-added intermediates or end-products (e Silva et al., 2006). In chemical terms, terpenes are organic hydrocarbons which are categorised based on the number of isoprene units (C_5H_8)_n in their molecule (Mewalal et al., 2017). Today, the industrial-scale production of terpenoid feedstocks is achieved either by tapping trees or via extraction from the by-products of the Kraft pulp industry (Behr and Johnen, 2009).

2.2. Theoretical lens

Operations Management scholars conduct multi-tier SC investigations aiming to test and refine sustainability theory and practice (Walker et al., 2014). Furthermore, the circular exploitation (e.g. reuse, remanufacture, recycle) of waste streams and renewable feedstocks is a strategic objective for sustainable SC management (Mangla et al., 2018), intending to support the development of restorative production systems through optimising product life cycles, material flows and waste streams (Genovese et al., 2017). In this regard, circular supply networks advance sustainable SC management research and practise via promoting triple bottom line sustainability (Geissdoerfer et al., 2018). This study is thus positioned in the sustainable SC management field, specifically focusing on advancing theory and informing practise in the design of circular supply networks defined by renewable chemical feedstocks.

This research adopts the systems view as theoretical lens following the general propensity to acknowledge SCs as systems (Caddy and Helou, 2007) with corresponding design, analysis and management ramifications (Carter et al., 2015). In particular, the systems view allows for the consideration of the various interrelated elements that collectively affect the viability of renewable chemical feedstock-driven SCs. The fundamental theme areas which are employed for the analysis, design and management of SC

systems are based on the work of [Srai et al. \(2018\)](#). These theme areas of analysis are: (i) renewable feedstock and substrate system definition ([Böhmer et al., 2012](#)); (ii) technology options for substrate conversion to intermediates ([Xu et al., 2012](#)); (iii) market and economic potential evaluation of intermediates or end-products ([Vispute et al., 2010](#)); and (iv) system of systems mapping for value creation and viability assurance ([Paulo et al., 2013](#)). The abovementioned theme areas are typically considered in isolation in the extant literature. In this regard, we adopt a systems view for renewable chemical feedstocks to enable the inclusive exploration of alternative network configuration opportunities, as illustrated in [Fig. 1](#).

The systems view consists of four interlinked theme areas, each requiring specific data and analysis approaches to devise circular value chains enabled by renewable chemical feedstocks. Initially, statistical and geospatial analysis of “Renewable Chemical Feedstock” alternatives can guide the techno-economic assessment of potential compounds to be exploited in a circular economy context. Afterwards, experts’ opinion and technical feasibility studies of available “Technology and Processing” options can inform stakeholders about existing industrial production routes or necessitated chemical conversion pathways. “Market” analysis and relevant evaluation techniques can then indicate petroleum-based intermediates or end-products that could be replaced by value-added equivalents derived from renewable compounds. An ongoing assessment of the “Value and Viability” of the configured networks can support the management of operations across end-to-end circular SCs.

2.3. Research approach

The nature of this research is exploratory in order to allow the development and testing of new theories ([Barratt et al., 2011](#)). To that end, this study relies upon inductive logic and diverse qualitative data to develop a framework which can be validated and verified ([Eisenhardt and Graebner, 2007](#)). The approach elaborated to address the research queries articulated in this study uses both primary and secondary evidence as the object of scrutiny. More specifically, the employed research approach combines both theory-based ([Eisenhardt and Graebner, 2007](#)) and practice-derived ([Yin, 2009](#)) evidence to investigate the contemporary phenomenon of circular supply networks defined by terpenoid renewable chemical feedstocks, both in-depth and within its real-life context. To generate synthesising arguments for the circular SC management domain this research relies upon three methodological stages: (i) a review of the extant literature ([Tranfield et al., 2003](#)); (ii) a supply network mapping technique ([Tsolakis and Srai, 2018](#)); and (iii) experts’ opinion ([Gephart, 2004](#)). The discussed case study further assists in establishing the foundations for theory development ([Rowley, 2002](#)).

At the first research stage, we synthesised the dispersed literature on renewable chemical feedstocks to obtain symbolic data (e.g. text) about the considered four theme areas of analysis. The case of terpenes was selected as a promising exemplar case for a range of reasons including ([Behr and Johnen, 2009](#)): significant availability of these compounds from diverse sources; promising upscaling production potential; structural similarity of terpenes to unsaturated hydrocarbons; eligibility to alternative processing pathways; and non-competitive nature with food production. However,

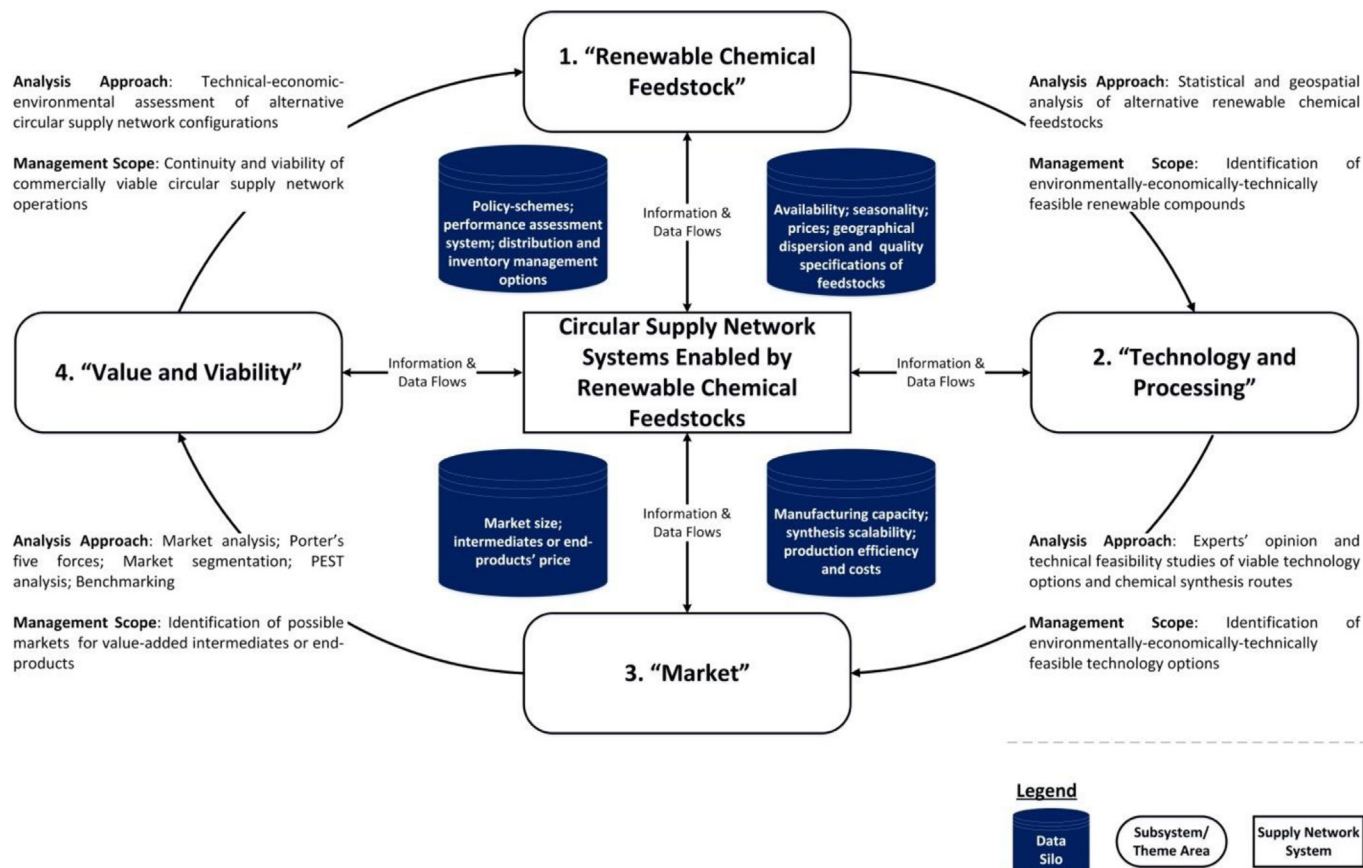


Fig. 1. Circular supply networks enabled by renewable chemical feedstocks – A systems view (based on [Srai et al., 2018](#)).

terpenes have not been comprehensively studied in the SC literature. To this effect, the long-standing documented use of terpenes in major manufacturing industries like biofuels (Meylemans et al., 2012), fine chemicals (Monteiro and Veloso, 2004) and polymers (Bähr et al., 2012) could inspire circular network (re)configuration opportunities applicable to other production sectors.

At a second research stage, following the work by Srail and Christodoulou (2014), we mapped potential circular network configurations for key identified terpenes, driven by the four theme areas of analysis. The interlinks between the theme areas increase managerial awareness and could inspire better practices in terms of creating circular SC functions (Ali et al., 2017). The resulting conceptual network structure was guided by the literature review on terpenes to foster the understanding about key constructs of circular supply networks defined by terpene-based compounds.

At a third research stage, primary data was identified through interviews with selected subject matter experts who provided testimonies and inductive reasoning; the primary evidence was used to formulate more abstract generalisations to the circular SC management theory (McAbee et al., 2017). Semi-structured interviews were conducted with a panel of 14 experts with diverse backgrounds. This type of consensus enabled a reduction in bias and an increase in the reliability of the retrieved data and the research findings. An experts' panel engagement was used to test data accuracy as well as to refine and validate the derived circular supply network mapping results. The updated SC mapping findings were used in subsequent iterations of data collection to identify any remaining uncertainties regarding the case of terpenes. The research methodology flowchart is depicted in Fig. 2.

2.4. Data collection and analysis

Data regarding the case of terpenes was collected from both primary and secondary sources, including: (i) literature; (ii) interviews; and (iii) academic workshop. The data analysis involved SC mapping techniques across the four identified theme areas of focus.

Firstly, to provide academic rigour and theoretically ground this research we utilised peer-reviewed scientific works. The criteria of the literature search are summarised in Fig. 2. The grey literature provided industry relevance and assisted in realising practical inferences. The qualitative research focused on the single, yet wide-ranging, case of terpenes to develop a common SC network structure that may be tested on other classes of renewable compounds.

Secondly, the academic and grey literature acquisition was directed and validated by subject matter experts to refine and validate the results and to identify gaps and redundancies in the criteria of the resulting maps. Overall, 14 semi-structured interviews were conducted involving academic and industry informants to reduce bias and increase the reliability of the gathered data and findings (Eisenhardt and Graebner, 2007). More precisely, 11 in-person and 3 telephone interviews were organised. The selection of the experts – affiliated to distinguished university institutions and multinational organisations – was based on their long-term involvement in empirical and experimental research related to renewable chemical feedstocks and SC management. Table A1 in the Appendix sets out the specific expertise of the 14 informants and further summarises key provided insights. To harness experiences and gain insights based on the four theme areas of analysis, two categorical levels of experts were recognised (Fig. 3), namely:

- i. Systems engineering level – informed by experts in the fields of renewable chemical feedstocks (3 experts), pharmaceuticals (1 expert), and systems engineering (2 experts), for gaining

insights regarding the technology and processing, and the market theme areas.

- ii. Technical and technology level – informed by experts in the fields of chemistry (3 experts), chemical engineering (4 experts), and biology and biochemistry (1 expert), for attaining insights regarding the renewable chemical feedstock, and the value and viability theme areas.

The number of interviewed informants is deemed appropriate as they represent a considerable share of the globally available expertise on renewable chemical feedstocks investigating a range of relevant topics, including: development of novel terpene-related chemistry; chemical engineering aspects including reactor design for processing terpenes; promising chemical and microbial synthesis pathways for terpenes; production upscaling considerations relevant to terpenes; supply network configurational designs; and operations management implications. In addition, most of the experts had been successful in six out of the twelve projects recently granted by the EPSRC with the aim to promote the scientific and industrial prospects of renewable chemical feedstocks in the United Kingdom. Therefore, the range and complementarity of the informants' expertise, based on the theoretical lens of this research, is judged sufficient to propose a network structure for circular SCs defined by terpenoid feedstocks. Moreover, the inclusion of informants with diverse areas of expertise results in a proposed network that further allows the ex-ante economic viability and environmental impact assessment of alternative renewable compounds.

Thirdly, a multi-stakeholder workshop served to triangulate the gathered data, build consensus, and refine and validate the collective outputs to gain greater insights. In particular, during the workshop, the mapping results were presented to the panel of experts so as to stimulate comments and constructive criticism.

3. Renewable chemical feedstocks: the illustrative case of terpenes

The increasing discourse regarding sustainability in manufacturing has led to an upsurge in renewable materials (Zhu et al., 2016). To that end, this research emphasises the design of value network operations that ensure the industrial and commercial potential of terpenes. In the subsections that follow an analysis and mapping of terpenes is provided, based on each of the four theme areas of analysis identified in this study.

3.1. 'Renewable chemical feedstock' theme area

Generally, four main sourcing options of terpenes are identified: (i) naturally occurring terpenes which are extracted from bio sources (e.g. artemisinin extracted from *Artemisia annua*); (ii) chemically extracted terpenes as by-products from biomass processing industries (e.g. pinene extracted from turpentine which in turn is a by-product of the Kraft process used in the pulp and paper industry); (iii) synthetically produced terpenes through specialised microbes (e.g. yeast being used to produce farnesene from glucose extracted from sugar cane); and (iv) terpenes present in unsustainable sources (e.g. squalene obtained from deep-sea shark liver).

A variety of natural sources of terpenes is reported (Davies et al., 2015). Evergetis and Haroutounian (2014) studied herbal materials from 22 different plant species of the Apiaceae family and reported the isolation of terpene-based fine chemicals from the obtained essential oils. Major extracted terpenes included α -pinene and limonene in the form of racemic mixtures; sesquiterpenes like γ -elemene and α -farnesene were also documented as potential isolation targets. Fuchs and Schwab (2013) reported the

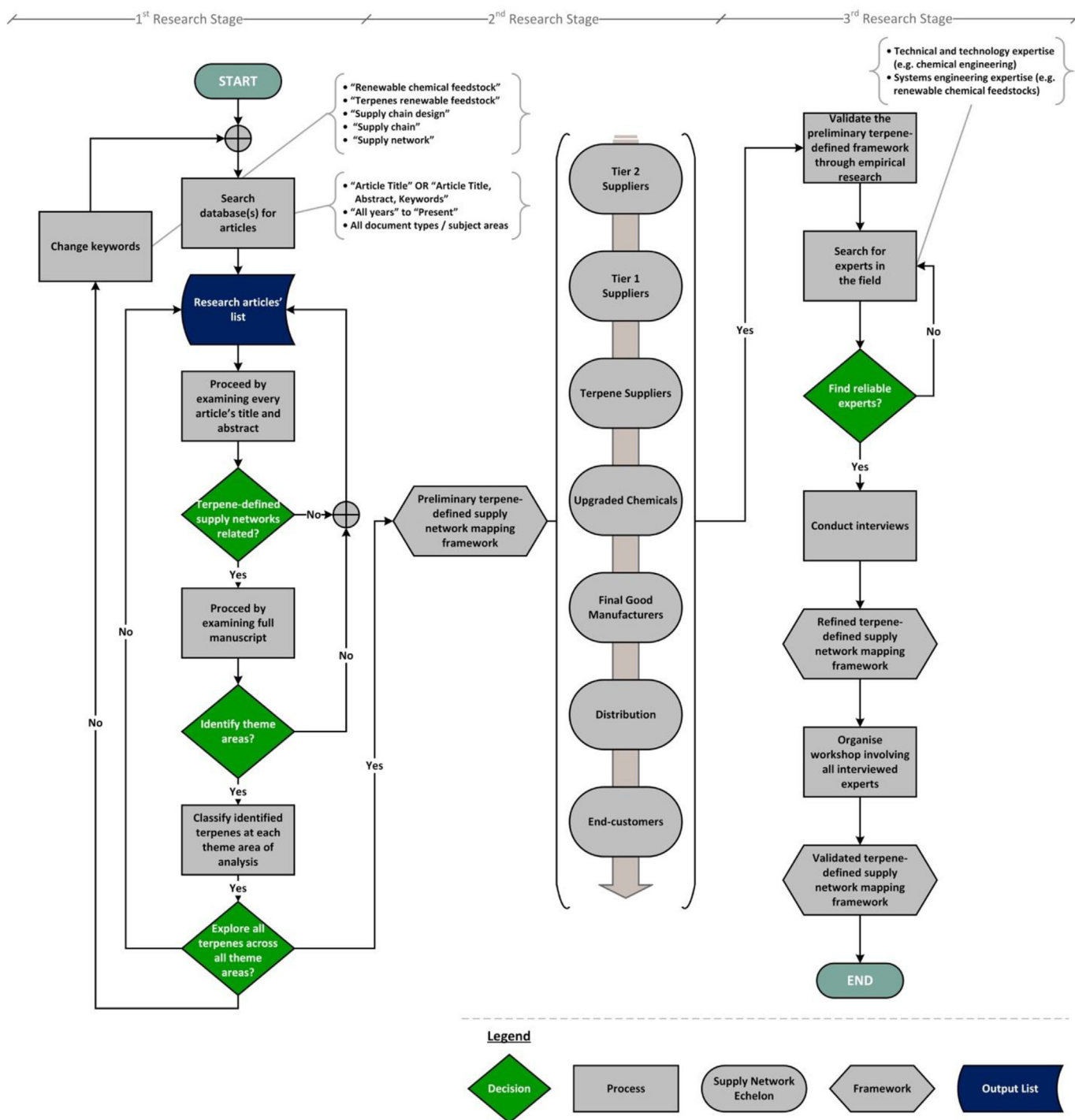


Fig. 2. Research methodology flowchart.

epoxidation of limonene and γ -terpinene which can be transformed in different chemical substrates thus enabling novel industrial applications. Kotan et al. (2007) observed 21 oxygenated monoterpenes as widespread components of plant essential oils focusing specifically on nerol, while Marzec et al. (2010) reported the isolation of α -terpinene from a variety of plant sources. Monteiro and Veloso (2004) also summarised major terpene-based components obtained from plants including: (i) eugenol from clove; (ii) geraniol from geranium; (iii) citral from lemongrass and citrics; and (iv) citronellal in citronella. In this vein, Schwab et al.

(2013) documented the presence of terpenes in essential oils like asmenthol in peppermint, linalool in lavender, citral in lemongrass, citronellal in citronella, and geraniol in geranium. In addition, Ajikumar et al. (2010) and Davies et al. (2015) reported the isolation of taxol from the bark of the Pacific yew.

Furthermore, crude sulphate turpentine is recognised as the most important source of terpenes (Behr and Johnen, 2009). Erman and Kane (2008) reported the extraction of α - and β -pinene from crude sulphate turpentine found in waste streams of paper and pulp mills. The authors reported that the ratio of α - and β -pinene in

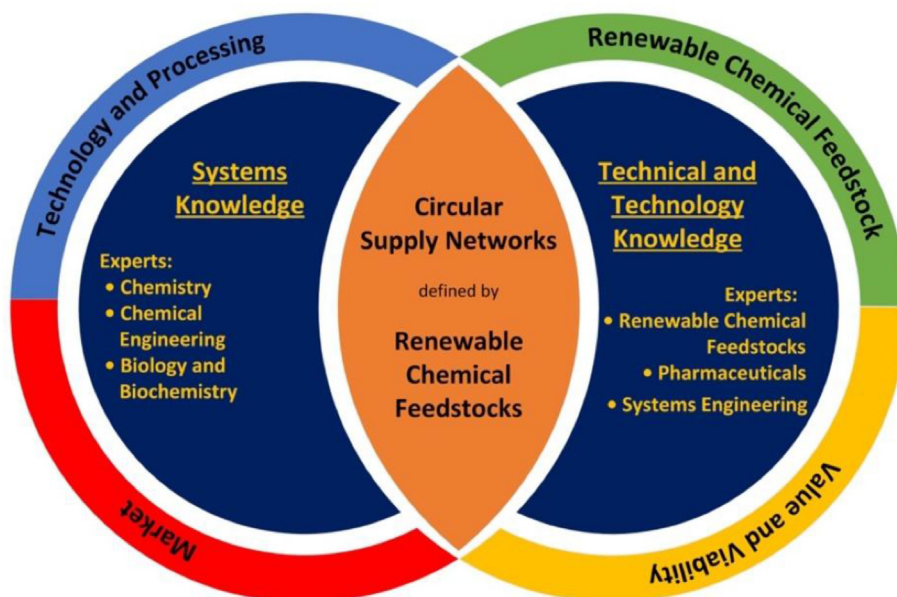


Fig. 3. Range and complementarity of experts involved in academic interviews.

crude sulphate turpentine depends on factors like tree species, regional and seasonal factors. Yang et al. (2013) recorded the industrial scale production of α -pinene by either tapping trees (gum turpentine) or as a component of crude sulphate turpentine, confirming the findings of Pakdel et al. (2001) who documented α - and β -pinene as significant by-products of pine wood distillation. The latter authors also discussed the significant yields of terpineol through the hydration of crude turpentine oil.

More recently, the potential of microbial synthesis and consolidated bioprocesses to extract terpenes from agricultural, forest and municipal waste products has drawn increased research interest. These production routes could contribute towards the sustainable manufacturing of products currently relying on non-renewable sources. For example, Yang et al. (2013) developed the microbial synthetic pathway of α -pinene in *Escherichia coli*. Additionally, Davies et al. (2015) reviewed heterotrophic and photoautotrophic microbial platforms to produce terpenes in large scales, further arguing that marine photosynthetic microbes hold potential for industrial scale production as they grow in salt water without requiring exogenous carbohydrate feedstocks. Moreover, Zhang et al. (2014) described the microbial synthesis of sabinene in a laboratory environment, while Peralta-Yahya et al. (2011) reported the engineering of microbial platforms to produce bisabolene.

Terpenes can be also derived in smaller quantities from a variety of origins including unsustainable sources like shark liver oil (Rocha et al., 2014) and crude oil (Gordillo et al., 2009). Table 1 provides a taxonomy of the main identified feedstock sources and potential extracted terpenes.

The wide range of sources of terpenes implies different capacity availabilities and extraction costs along with different levels of environmental impact for the related processes. Especially, environmental concerns such as high-energy use during distillation processes and exploitation of deep-sea sharks for the production of squalene and squalane highlight the varying viability of different terpenoid feedstock sources. Furthermore, in case renewable chemical feedstocks are extracted from by-products of other industries the possible volumes are dependent on the different industries' performance. Independent sources are bound by other feasibility constraints and concerns such as land availability and

potential competition with food sources. Synthetically produced terpenes are bound by similar constraints as they require biomass from either dependent (e.g. municipal waste) or independent (e.g. glucose extracted from sugar cane) sources.

3.2. 'Technology and processing' theme area

In literature, terpenes are often linked to marketable products without specifying the processing routes and conversion pathways that every terpene-based compound would have to undergo prior to its commercialisation. Despite the wide variety of terpenes, certain main processes emerge in literature for the final consolidation of the compounds; however, these processes are adapted to provide the optimal performance in every renewable chemical feedstock instance. In this context, in the application of the technological processing analysis to terpenes we consider four conversion steps, namely: (i) biomass processing; (ii) terpene extraction and production; (iii) terpene purification; and (iv) terpene valorisation. The process map in Fig. 4 illustrates the main processing steps required to convert naturally available terpenoid feedstocks to value-added intermediate chemical compound options. Determining the combination and order of conversion processes for terpenes becomes increasingly complex downstream the SC as the variety of possible commercial products increases.

The technology and processing map enables the identification of technological barriers and linkages that need to be developed to unlock specific added-value derivatives. Furthermore, as the aim of this research is to determine sustainable substitutes for petrochemicals, environmental considerations such as carbon footprint, freshwater appropriation, use of toxic and hazardous chemicals, and competition with food resources, also need to be considered for each processing pathway. Below, the technology and processing pathways for terpenes are discussed while a taxonomy of relevant and up-to-date research efforts is provided.

3.2.1. Biomass processing

Biomass processing is vital for extracting raw materials that contain significant volumes of terpenoid compounds. The choice of the extraction technique may profoundly impact the properties of

Table 1
Feedstock sources and major extracted terpenes.

Source	Major extracted terpene	References
1. Plant essential oils	1.1 α - and β -pinene (coniferous trees)	Evergetis and Haroutounian (2014); Fuchs and Schwab (2013); Kotan et al. (2007); Marzec et al. (2010)
	1.2 limonene (citrics)	Monteiro and Veloso (2004); Vieira et al. (2018)
	1.3 nerol	Lu and Wang (2018); Kotan et al. (2007)
	1.4 eugenol (clove)	Monteiro and Veloso (2004)
	1.5 geraniol (geranium)	Monteiro and Veloso (2004); Schwab et al. (2013)
	1.6 citral (lemongrass, citrics)	Monteiro and Veloso (2004); Schwab et al. (2013)
	1.7 linalool (lavender)	Pereira et al. (2018); Schwab et al. (2013)
	1.8 camphene	Benelli et al. (2018); Monteiro and Veloso (2004)
	1.9 citronellal (citronella, eucalyptus)	Monteiro and Veloso (2004); Schwab et al. (2013)
	1.10 taxol (Pacific yew)	Ajikumar et al. (2010); Davies et al. (2015)
	1.11 artemisinin (sweet wormwood)	Davies et al. (2015); Tellez et al. (1999)
2. Crude sulphate turpentine	2.1 α - and β -pinene	Behr and Johnen (2009); Erman and Kane (2008); Pakdel et al. (2001); Yang et al. (2013)
3. Microbial production	2.2 terpineol	Behr and Johnen (2009); Pakdel et al. (2001)
	3.1 carotene	Davies et al. (2015)
	3.2 astaxanthin	Davies et al. (2015)
	3.3 α -pinene	Yang et al. (2013)
	3.4 sabinene	Zhang et al. (2014)
	3.5 bisabolene	Peralta-Yahya et al. (2011)
4. Non-sustainable sources	3.6 farnesene	Davies et al. (2015)
	4.1 squalene (deep-sea shark liver)	Rocha et al. (2014)
	4.2 isoprene (crude oil)	Gordillo et al. (2009)

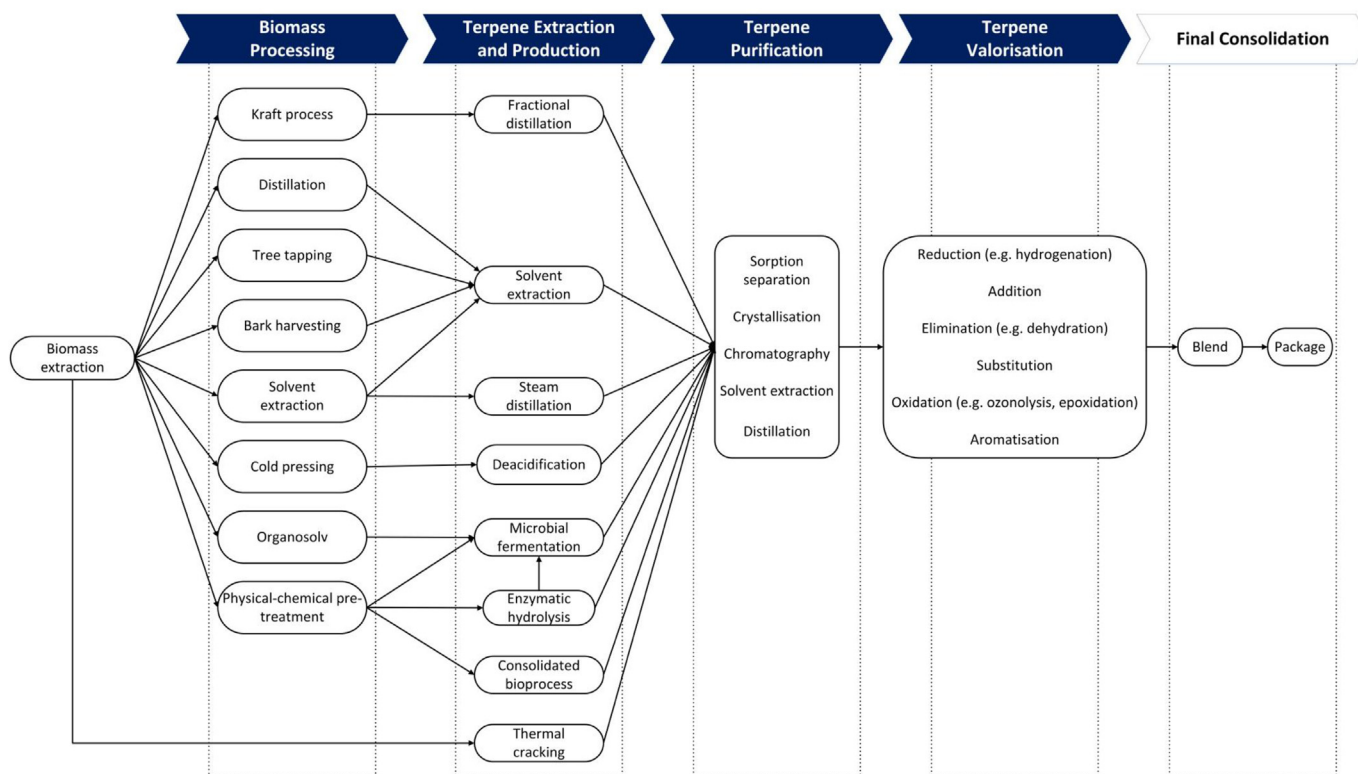


Fig. 4. Terpenes' technology and processing pathways.

the derived terpenes, hence affecting the synthesis of the intermediate or end-products. Initially, until the 1950s, terpenes were being harvested from natural sources via tree tapping to obtain turpentine (Erman and Kane, 2008). Later, developed countries devised new methods for the recovery of crude sulphate turpentine from the waste streams of paper mills (Pito et al., 2009). Nowadays, Kraft processing is reported as the primary method to extract crude sulphate turpentine (Knuuttila, 2013), a major by-product in paper and chemical pulp manufacturing (Behr and Johnen, 2009). More

specifically, in the Kraft process, wood chips of dead trees are partly solubilised (Firdaus et al., 2011) and crude sulphate turpentine is obtained from the condensate of the waste gas; crude sulphate turpentine from Kraft paper mills normally contains fatty acids and gum resin thus necessitating a cleaning treatment for the removal of heavy products (Roberge et al., 2001).

Davies et al. (2015) provided examples of tepenoid feedstocks being isolated during bark harvesting of the Pacific yew. Chemat et al. (2012) reported the extraction of essential oils rich in

terpenes isolated from the bark of the Western yew. [Monteiro and Veloso \(2004\)](#) reported that essential –juice– oils are usually extracted from plants (e.g. leaves, stems, flowers, fruits) by cold expression. In particular, [Vázquez et al. \(2009\)](#) reported that olive oil, known for its pleasant flavour provided by major C5 compounds, is commercially obtained by cold pressing. Moreover, [Wilbon et al. \(2013\)](#) provided a review regarding recent advances in the field of renewable bio-based monomers and polymers from natural resources and further reported the utilisation of a novel pulping technique, called organosolv, to produce rosin-based graft copolymers. Notably, the biomass sources of terpenes need to be analysed in terms of their physico-chemical quality specification nexus and, depending on their properties, have to undergo a pre-treatment process for preparing the biomass for the extraction of terpenes ([Zhang et al., 2013](#)). [Table 2](#) summarises the technology options for processing biomass sources of terpenes.

3.2.2. Terpene extraction and production

Terpene extraction is used either to obtain terpenes from biomass or to increase the purity of a terpene-based mixture. For example, [Vázquez et al. \(2009\)](#) studied the deacidification of crude olive oil and suggested the process as appropriate to extract precursors of important terpenes from vegetable oils. [Park et al. \(2013\)](#) reported the production of isoprene from carbohydrates by microbial fermentation. Similarly, [Zhang et al. \(2014\)](#) explored the ‘green’ and sustainable production of sabinene, one kind of monoterpene used as a component for the next generation of aircraft fuels, through microbial fermentation using engineered *Escherichia coli* strains. [Yang et al. \(2013\)](#) documented the microbial fermentation process as appropriate to: (i) convert renewable resources into monoterpene products; and (ii) optimise the biosynthesis pathway of α -pinene into *Escherichia coli*. [Hong and Nielsen \(2012\)](#) also supported the use of microbial fermentation for the extraction of terpenes used in the production of fuels, specifically discussing the case of farnesene which is used as a biodiesel component. [Peralta-Yahya et al. \(2011\)](#) optimised the microbial fermentation conditions to improve the productivity of large quantities of biosynthetic bisabolene for complete fuel property analysis.

Hydrolysis is also used to extract terpenes from natural oils ([Yao and Tang, 2013](#)). [Pourbafrani et al. \(2013\)](#) reported the use of acid hydrolysis in large biorefineries for the recovery of terpenes, as for example limonene from citrus waste. [Idem et al. \(1996\)](#) studied terpene-based products obtained from the thermal cracking of canola oil. Common terpenes for current steam crackers were also reported by [Zimmermann and Walzl \(2009\)](#). [Table 3](#) summarises the identified technological processes for extracting and producing terpenes.

Apart from the established extraction processes for terpenes indicated in [Table 3](#), other less common solutions include: distillation; molecular distillation; chromatography; microwave extraction; ultrasound assisted extraction; solvent extraction/liquid-liquid extraction; sorption separation; supercritical fluid extraction; and membrane separation.

3.2.3. Terpene purification

Terpenes obtained through extraction/production processes are often characterised by inadequate purity levels for commercial applications. In this regard, an additional purification step is required. Often, though, the extraction and purification steps are integrated in practice. Indicatively, solvent extraction and distillation are normally used to both extract terpenes from plant material and increase the purity of a terpene-based compound mixture.

Solvent extraction is a common method for obtaining purified terpenoid content from plants’ essential oils ([Monteiro and Veloso, 2004](#)). [Liu et al. \(2011\)](#) studied a large-scale solvent extraction and purification method of the sesquiterpene lactone artemisinin from *Artemisia annua*, a common type of wormwood. [Martins et al. \(2016\)](#) evaluated novel ionic liquids used either as solvents for extraction or as entrainers in separation processes involving terpenes. [Xu et al. \(2000\)](#) reported the synthesis of adsorbents with high selectivity for terpene lactones that could be used in purification of ginkgo leaf extracts at industrial scale applications.

Furthermore, [Bajer et al. \(2016\)](#) developed a hydrodistillation process for the separation and determination of highly purified terpenes from allspice berries. [Behr and Johnen \(2009\)](#) reported the extraction and purification of α -pinene, β -pinene, 3-carene, limonene, and camphene from turpentine through fractional distillation, under low pressure. [Firdaus et al. \(2011\)](#) described the extraction of α - and β -pinene from the resinous sap of pine trees through steam distillation. The latter process of distilling resinous sap from pine or conifer trees provides purified pinenes which can undergo a multitude of chemical reactions to manufacture valuable monomeric compounds ([Wilbon et al., 2013](#)). [Meylemans et al. \(2012\)](#) informed that for the case of terpene-based mixtures, fractional distillation of turpentine is an energy consumptive step towards the isolation of pure compounds. Different distillation techniques are reported for the extraction of purified terpenes from different essential oils. For example, steam distillation is typically used for the processing of peppermint and lemongrass oil whereas vacuum distillation is suggested for the case of pine and orange oil terpenes.

[Lu et al. \(2003\)](#) proposed a high-speed counter-current chromatography technique for the preparative separation and purification of squalene from microalgae. Finally, [Reed and Rilling \(1975\)](#) reported the experimental purification of prenyltransferase from chicken liver through crystallisation. The study represents the first documented preparation of a stable crystalline enzyme of sterol and terpene biosynthesis. In [Table 4](#) the main processes for purifying terpenes are briefly tabulated.

3.2.4. Terpene valorisation

Terpene valorisation is used to transform the chemical structure of terpenes to allow their use in various commercial applications or to enable further processing and conversion steps. Research in this field seeks to: (i) identify novel pathways to convert terpenes into useful compounds; and (ii) devise technological solutions that enable the upscaling of terpenoid synthesis pathways to promote commercial viability. For example, [Corma et al. \(2007\)](#) in their

Table 2
Technology and processing options for attaining natural –biomass– sources of terpenes.

SC Level	Technology/Process	References
1. Biomass processing	1.1 Tree tapping	Erman and Kane (2008) ; Neis et al. (2018)
	1.2 Kraft processing	Behr and Johnen (2009) ; Firdaus et al. (2011) ; Knuuttila (2013) ; Pito et al. (2009) ; Roberge et al. (2001)
	1.3 Bark harvesting	Chemat et al. (2012) ; Davies et al. (2015)
	1.4 Cold pressing	Monteiro and Veloso (2004) ; Vázquez et al. (2009)
	1.5 Organosolv	Tang et al. (2017) ; Wilbon et al. (2013)
	1.6 Pre-treatment	Zhang et al. (2013)

Table 3

Technology and processing options for extracting and producing terpenes.

SC Level	Technology/Process	References
2. Terpene extraction	2.1 Deacidification	Vázquez et al. (2009)
	2.2 Microbial fermentation	Hong and Nielsen (2012); Park et al. (2013); Peralta-Yahya et al. (2011); Yang et al. (2013); Zhang et al. (2014)
	2.3 Acid/enzymatic hydrolysis	Hua et al. (2018); Pourbafrani et al. (2013); Yao and Tang (2013)
	2.4 Thermal cracking	Idem et al. (1996); Silva et al. (2017); Zimmermann and Walzl (2009)

Table 4

Technology and processing options for purifying terpenes.

SC Level	Technology/Process	References
3. Terpene purification	3.1 Solvent extraction	Liu et al. (2011); Martins et al. (2016); Monteiro and Veloso (2004); Xu et al. (2000)
	3.2 Distillation	Bajer et al. (2016); Behr and Johnen (2009); Firdaus et al. (2011); Meylemans et al. (2011, 2012); Wilbon et al. (2013)
	3.3 Chromatography	Gao et al. (2018); Lu et al. (2003)
	3.4 Crystallisation	Reed and Rilling (1975)

review identified a plethora of transformation processes as important routes for the valorisation of functionalised terpenes. Knuuttila (2013) reported the purification of crude sulphate turpentine from all its sulphur compounds through hydrogenation, in a single reaction phase. In addition, Monteiro and Veloso (2004) provided a review of the catalytic conversion of terpenes into fine chemicals and discussed the reduction of citronellal with isopropanol to citronellol.

Firdaus et al. (2011) described the solvent and radical initiator-free addition of thiols to limonene and β -pinene as a simple approach to obtain a wide range of functionalised renewable monomers. Monteiro and Veloso (2004) also reported the hydration of α -pinene to camphene to produce camphor, while Pakdel et al. (2001) studied the hydration of α -pinene to obtain high yields of α -terpineol. Pito et al. (2009) studied the methoxylation of α -pinene and observed high yields of α -terpinyl methyl ether and other terpenes as by-products. Schwab et al. (2013) documented hydration as an appropriate biotransformation process of terpenes that enables the large-scale production of valuable chemicals. Firdaus et al. (2011) also reported the partial dehydration of cistein hydrate into terpineol to yield the most important monocyclic monoterpene alcohol, while Monteiro and Veloso (2004) reviewed operative dehydrogenation mechanisms of various terpenes such as limonene, 3-carene, and α -pinene to produce p-cymene. Furthermore, Roberge et al. (2001) investigated the dehydrogenation of α -pinene to p-cymene that leads to stable end-products.

Towards increased sustainability, biotechnological approaches to terpene valorisation demonstrate potential for use in biorefineries. However, many of these processes, like bio-oxidation, still have low transformation rates and high production costs thus requiring further research to unlock the potential of such technologies (Bicas et al., 2009). In this context, Behr and Johnen (2009) provided a review of the aromatisation potential of myrcene as a building block for sustainable chemistry. The authors also reviewed a variety of possible downstream products of myrcene through hydrochlorination and various other processing routes. Monteiro and Veloso (2004) also reviewed terpene oxidation methods to produce important molecules. Park et al. (2013) reported the epoxidation of limonene to produce inexpensive and readily available bio-sourced monomers.

Behr and Johnen (2009) described the chemical modification of terpenes using reactions such as aromatisation, while Laitinen et al. (2012) focused on the conversion of α -limonene and pinene to p-cymene by catalytic aromatisation. Schwab et al. (2013) supported the enzymatic aromatisation of terpenes to enable their convenient and cost-effective large-scale valorisation. Tracy et al. (2009)

detected cymene as a product of limonene aromatisation.

Furthermore, Firdaus et al. (2011) reported the industrial production of camphene by isomerisation of α -pinene that is then used as a value-added intermediate in the chemical industry. Monteiro and Veloso (2004) stressed the isomerisation of citronellal to isopulegol, a terpene-based alcohol used as an intermediate in: (i) the synthesis of menthols; and (ii) the isomerisation of α -pinene to monocyclic terpenes and alcohols with α -terpineol as the main product. Similarly, Schwab et al. (2013) reviewed catalytic conversions of terpenes into fine chemicals, reporting amongst others isomerisation as a valuable biotransformation reaction. Wilbon et al. (2013) indicated that the isomerisation of pinene leads to a plethora of interesting monoterpenes like for example myrcene.

Moreover, Firdaus et al. (2011) provided a suitable tool for the optimal polymerisation of difunctional monomers, while Laitinen et al. (2012) investigated the optimisation of the emulsion polymerisation process for the synthesis of α -methylstyrene monomer with the aim to increase the resulting dry solids content and decrease the amount of unreacted monomer. Park et al. (2013) reported that the copolymerisation of difunctional monomers results in increased reaction rates and shortened induction periods of the photopolymerisation of such monomers. Likewise, Quilter et al. (2017) investigated the polymerisation of a terpene-derived lactone and evaluated the potential application of the derived polymer as a bio-based alternative to the petrochemically derived ϵ -caprolactone. Wilbon et al. (2013) reviewed polymerisation and copolymerisation processes of terpenes, such as pinene, limonene, and myrcene, towards renewable bio-based monomers and polymers. Yao and Tang (2013) reviewed opportunities and challenges related to the controlled polymerisation of terpenes to produce high performance polymers with controlled molecular weight, functionalities, and architectures. The main technological processes for the valorisation of terpenes are highlighted in Table 5.

3.3. 'Market' theme area

Terpene-based products have various commercial applications including insecticides (Evergetis and Haroutounian, 2014), detergents (Gordillo et al., 2009), anti-oxidant agents (Marzec et al., 2010), solvents (Roberge et al., 2001), tobacco cooling agents (Tan and Zou, 2001), fuel (Tracy et al., 2009), and polymers (Erman and Kane, 2008) amongst others. The variety of products and commercial markets implies different demand volumes, price points and price elasticities for diverse terpene-based products. Below, some of the most important applications of terpenes are discussed.

To begin with, flavours and fragrances are the most common

Table 5
Technology and processing options for valorising terpenes.

SC Level	Technology/Process	References
4. Terpene valorisation	4.1 Reduction (e.g. hydrogenation)	Corma et al. (2007); Knuuttila (2013); Monteiro and Veloso (2004)
	4.2 Addition (e.g. hydration, methoxylation)	Corma et al. (2007); Firdaus et al. (2011); Monteiro and Veloso (2004); Pakdel et al. (2001); Pito et al. (2009); Schwab et al. (2013)
	4.3 Elimination (e.g. dehydration, dehydrogenation)	Corma et al. (2007); Firdaus et al. (2011); Monteiro and Veloso (2004); Roberge et al. (2001)
	4.4 Condensation	Corma et al. (2007); Murzin and Simakova (2013)
	4.5 Oxidation (e.g. ozonolysis, epoxidation)	Behr and Johnen (2009); Bicas et al. (2009); Corma et al. (2007); Monteiro and Veloso (2004); Park et al. (2013)
	4.6 Aromatisation	Behr and Johnen (2009); Corma et al. (2007); Laitinen et al. (2012); Schwab et al. (2013); Tracy et al. (2009)
	4.7 Isomerisation	Corma et al. (2007); Firdaus et al. (2011); Monteiro and Veloso (2004); Schwab et al. (2013); Wilbon et al. (2013)
	4.8 Polymerisation	Firdaus et al. (2011); Laitinen et al. (2012); Park et al. (2013); Quilter et al. (2017); Wilbon et al. (2013); Yao and Tang (2013)

fields of application for terpene-derived intermediates or end-products with Bauer et al. (2008) and Fahlbusch et al. (2012) providing a detailed description of such applications. More specifically, the organic chemical compounds which are used to produce flavours and fragrances include myrcene (Behr and Johnen, 2009), cymene (Gallezot, 2007a), limonene (Gallezot, 2007b), and carvone (Demidova et al., 2016). Especially, limonene is used as both a fragrance molecule and a precursor for other perfumes (Swift, 2004). For the synthesis of flavours and fragrances, menthol (Bhatia et al., 2008), citral (Behr and Johnen, 2009), and camphor (Stanfill et al., 2015) are the most used terpenes. Food flavours are reported to leverage the chemical aroma derived from the condensation of citral (Schwab et al., 2013). Monteiro and Veloso (2004) reported the preference of terpenes as flavour agents (e.g. citral) over synthetic substances since they are ingested and their odour and flavour are usually more sophisticated. Cymene is also used as an additive in fragrances and musk perfumes, and as a masking odour for industrial products (Roberge et al., 2001).

Furthermore, pharmaceuticals provide prosperous ground for the exploitation of terpenoid feedstocks as the latter are valuable and reactive intermediates capable of facilitating a wide range of reactions in pharmaceutical and organic chemistry. Some terpenes (e.g. artemisinin) have been extensively used in pharmaceuticals (Liu et al., 2011) while others demonstrate a potential for industrial exploitation within the industry (Wu et al., 2016). Indicative terpenes with application in pharmaceuticals include myrcene (Behr and Johnen, 2009) and camphor (Behr and Johnen, 2009). Various terpenes have been used to produce antibacterial and analgesic medications like menthol (Tan and Zou, 2001) and terpinene (Marzec et al., 2010). Kotan et al. (2007) determined the antibacterial activities of 21 oxygenated monoterpenes and concluded that nerol, linalool, terpineol and fenchol demonstrate related activity at a broad spectrum. Bach (2010) also reported the potent antibacterial effects of anethol, fenchone and camphene while Roberge et al. (2001) informed about the similar effects of cymene. Novel functions of plant-derived terpenes have also been discovered, such as the anti-cancer properties of taxol and the anti-malarial effects of artemisinin (Davies et al., 2015). Squalene (Lu et al., 2003) and terpinene (Marzec et al., 2010) can potentially strengthen the human body's immune system and decrease the risk of cancer forms; squalene and squalene are predominantly used as vaccine adjuvants (Allison, 1999). Natural or synthetic resins of terpenes are used in several pharmaceutical synthesis pathways of vitamins, as for example myrcene (Behr and Johnen, 2009), linalool (Sabogal-Guáqueta et al., 2016), and limonene (Negro et al., 2016).

Additionally, the use of terpenes in the production of polymers is a broad and on-going research field (Firdaus et al., 2011). Wilbon et al. (2013) provided a broad review of the progress made in

utilising terpenes in the production of polymers to date. Such terpenes are for example myrcene (Behr and Johnen, 2009), limonene (Behr and Johnen, 2009), and farnesene (Behr and Johnen, 2009). Cymene is used to produce terephthalic acid (Golets et al., 2013) which is a precursor to the polyester PET utilised in the manufacturing of apparel and bottles. Isoprene and geraniol are also used for the preparation of synthetic rubber (Davies et al., 2015) and plasticisers (Kojima et al., 2005), respectively. For the synthetic rubber industry, pinenes and pinanes are used as cost-effective polymerisation catalysts (Erman and Kane, 2008). Recent research also demonstrates the potential of new chemical synthesis routes for the industrial production of renewable and biodegradable plastics using terpenes (Quilter et al., 2017).

Experimental results also revealed the potential application of terpenes in jet fuels, diesel and tactical fuels (Davies et al., 2015). Promising terpenes include limonene (Meylemans et al., 2012), pinene (Davies et al., 2015), camphene (Meylemans et al., 2012), and farnesene (Davies et al., 2015). For the case of next generation jet biofuels and fuel additives, the hydrogenated form of limonene is preferred as it demonstrates favourable properties, i.e. low freezing point and immiscibility with water that enhance cold weather performance of fuels (Tracy et al., 2009). Farnesene (Millo et al., 2014) and bisabolene (Davies et al., 2015) were documented to be used as diesel replenishment fuels. Tracy et al. (2009) reported the potential use of myrcene and limonene as additives to diesel fuels as well.

Novel applications of terpenes are continuously reported in the academic and industrial literature as research in the field is on-going. Examples include squalene which is normally used as a moisturising or emollient agent in cosmetics and pharmaceutical formulations (Lu et al., 2003). Gordillo et al. (2009) investigated the processing of isoprene to yield terpene derivatives with possible applications in the cosmetics and detergents sectors. Limonene is also used as a solvent or ingredient in water-free cleansers (Bomgardner, 2011). Cymene is considered a valuable intermediate in the chemical industry as it is used as a solvent for dyes and varnishes, and as a heat transfer medium (Roberge et al., 2001). Menthol is the prominent compound in many tobacco products where it was first introduced as an additive in the 1920s (Kamatou et al., 2013). Camphor and geraniol (Licciardello et al., 2013), as well as myrcene (Behr and Johnen, 2009), are documented as active ingredients in branded insect repellents. Other repellents for insects, including mosquitoes and the American cockroach, are manufactured based on cineole (Klocke et al., 1987). In the cleaning agents' market, linalool (Nørgaard et al., 2014) is used due to its pleasant scent. In addition, camphor is used for the fabrication of explosives (Rylott et al., 2011).

Main opportunities and challenges of key markets for terpene-

based product offerings are appended in Table 6. The table summarises key considerations that may be relevant for assessing the markets for terpenes by providing a high-level understanding of the opportunities and challenges characterising these markets.

3.4. 'Value and viability' theme area

Provided that a terpene-based value chain is established, following the analysis in the first three theme areas, i.e. renewable chemical feedstock, technology and processing, and markets, corresponding key actions for every network echelon should be identified to guide the data gathering process and ensure value creation and viability. The key required actions per terpene value chain step are illustrated in Fig. 5.

The value and viability mapping framework summarises the data required to determine the commercial potential of a terpene-based supply network. Indicatively, the cost and price factors included in the framework enable a degree of economic viability determination. Likewise, the volume factors enable the identification of capacity bottlenecks across the supply network, along with the estimation of the maximum volumes attainable. Therefore, the proposed framework could support the viability analysis of terpene-based solutions in terms of both economic and environmental aspects.

Nevertheless, the provided value and viability mapping framework fails to account for the interaction between volume and price while it also does not fully consider any uncertainties regarding the gathered data. Furthermore, the framework does not address SC considerations from an end-to-end perspective and may not capture the full complexity of the renewable chemical feedstock landscape.

In terms of network relationships, the dimensions suggested by [Srai and Christodoulou \(2014\)](#), namely intra-firm, inter-firm and network governance, are not all valid for the case of terpene-based value networks. More specifically, the intra-firm dimension does not apply to the terpenes case as it relies on a focal firm. However, the geographic dispersion, network integration, identification of key suppliers and customers, and the identification of player network roles are recognised as important in understanding the commercial viability of prospective SCs.

4. Terpene-based circular value chains

The assessment of future-state industries and product-process supply network (re)configurations, emerging from renewable chemical feedstocks, requires that a clear network structure of

respective sustainable SCs is defined ([Seuring and Müller, 2008](#)). In line with the methodology presented in Section 2, this section captures potential archetypal product-process combinations and articulates an end-to-end network structure for SCs emerging from terpenes (subsection 4.1). Key uncertainties that influence the commercial value and viability of the respective networks are further highlighted (subsection 4.2).

4.1. Network structure

According to [Srai \(2017\)](#), emerging industrial SCs, like networks defined by renewable chemical feedstocks, should systematically capture material transformations, process technologies, enabling products and network actors. In this regard, Fig. 6 provides an integrated view of all potential nodes and linkages in a SC structure from a terpenoid feedstock perspective. The network structure enables the identification of SC (re)configuration options dictated by specific feedstock sources or existing markets seeking to utilise terpenes as sustainable raw material. Unstable network structures are also indicated like for example squalene which is extracted from deep-sea shark liver oil and isoprene which is produced from petrochemicals.

In a circular economy context, Tier 2 suppliers represent the natural system with significant discarded or wasted renewable feedstocks rich in terpenes. For example, surplus forestry biomass or unexploited municipal waste could be collected and processed to both mitigate environmental impact and unleash innovative business potential. Thereafter, Tier 1 suppliers possess the capabilities and technologies for the collection and primary processing of the often-bulky and inexpensive renewable feedstocks into concentrated extracts with untapped commercial potential. The geographical distribution and capacity constraints of Tier 2 and Tier 1 suppliers, in conjunction with the physico-chemical properties of renewable feedstocks, can have significant ramifications to the SC by requiring a transition from the established centralised network configurations to decentralised structures. Distribution and logistics operations upstream in the SC could be impacted as well.

Following that, terpene suppliers can process the concentrated extracts to derive a range of terpenes. Terpene suppliers are developing their proprietary platform technologies to explore the production of terpenes, tackle any production upscaling issues and demonstrate confidence in scalability. Examining the by-products derived during the synthesis of terpenes could reveal other compounds, though likely in lower volumes, with value-added potential. From a SC management perspective, the opportunity to engage suppliers of discarded feedstocks in circular network operations

Table 6
Key markets for terpene-based intermediates or end-products.

Market	Opportunities	Challenges	References
Flavours and Fragrances	<ul style="list-style-type: none"> High value 	<ul style="list-style-type: none"> Low volume Technical infeasibility to currently replace petrochemicals 	Bauer et al. (2008) ; Behr and Johnen (2009) ; Bhatia et al. (2008) ; Breitmaier (2006) ; Demidova et al. (2016) ; Fahlbusch et al. (2012) ; Gallezot (2007a; b) ; Monteiro and Veloso (2004) ; Roberge et al. (2001) ; Schwab et al. (2013) ; Stanfill et al. (2015) ; Swift (2004)
Pharmaceuticals	<ul style="list-style-type: none"> High potential for pharmaceutical molecules' formulation 	<ul style="list-style-type: none"> Non-competitive production cost compared to existing techniques Low volumes of petrochemicals in pharmaceuticals 	Allison (1999) ; Attard et al. (2018) ; Bach (2010) ; Behr and Johnen (2009) ; Breitmaier (2006) ; Davies et al. (2015) ; Kotan et al. (2007) ; Liu et al. (2011) ; Lu et al. (2003) ; Marzec et al. (2010) ; Negro et al. (2016) ; Roberge et al. (2001) ; Sabogal-Guáqueta et al. (2016) ; Tan and Zou (2001) ; Wu et al. (2016)
Polymers	<ul style="list-style-type: none"> High potential for renewable polymers 	<ul style="list-style-type: none"> Technical difficulties towards the industrial scale production of polymers 	Amulya et al. (2016) ; Behr and Johnen (2009) ; Brodin et al. (2017) ; Davies et al. (2015) ; Erman and Kane (2008) ; Firdaus et al. (2011) ; Golets et al. (2013) ; Kojima et al. (2005) ; Quilter et al. (2017) ; Wilbon et al. (2013)
Fuels	<ul style="list-style-type: none"> Exceptional volumetric net heat of combustion Low volatility Compatibility with existing fuel infrastructure 	<ul style="list-style-type: none"> Non-competitive supply and production routes 	Davies et al. (2015) ; Meylemans et al. (2012) ; Millo et al. (2014) ; Tracy et al. (2009)

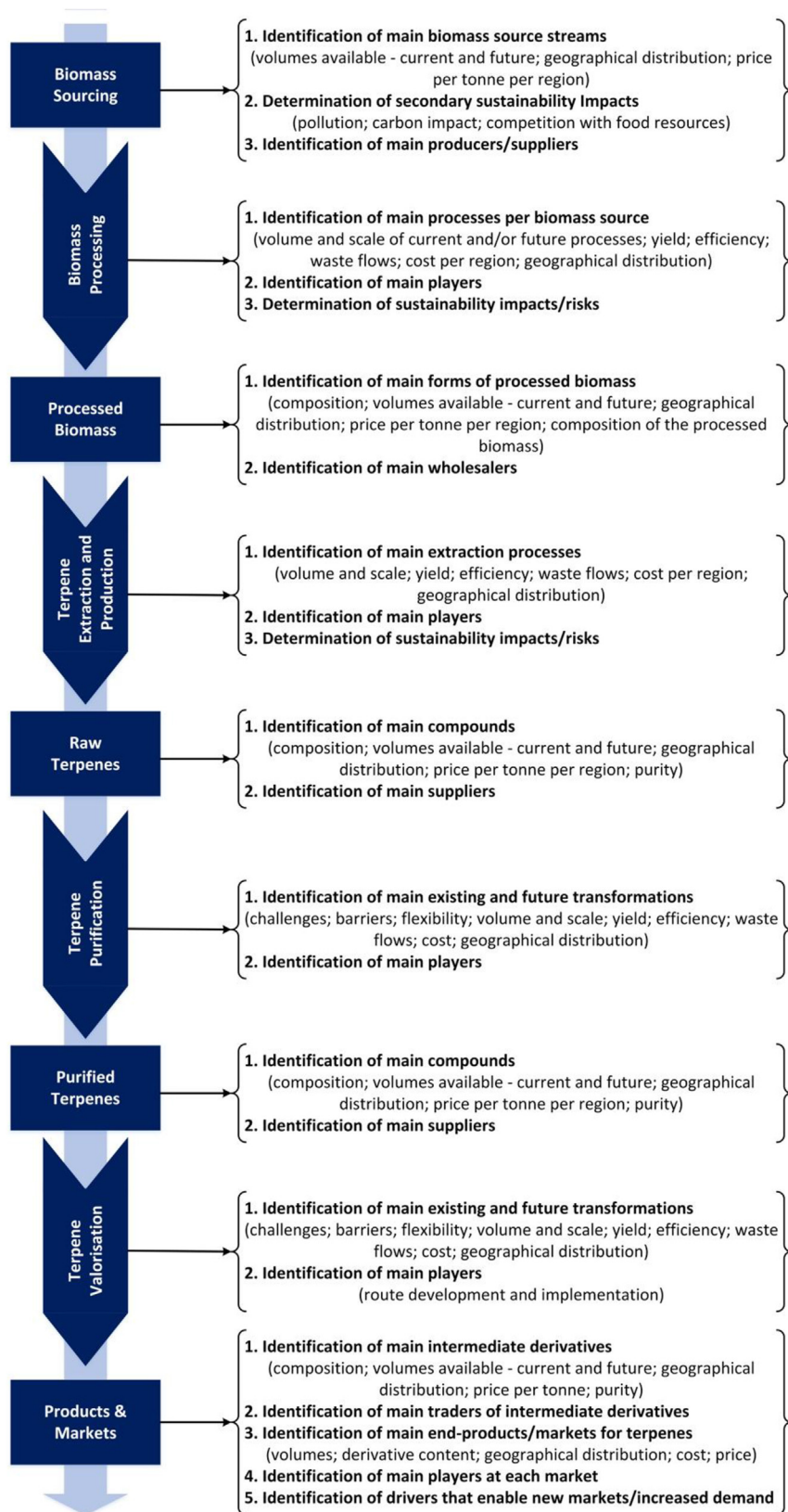


Fig. 5. Terpene-based supply network value and viability mapping framework.

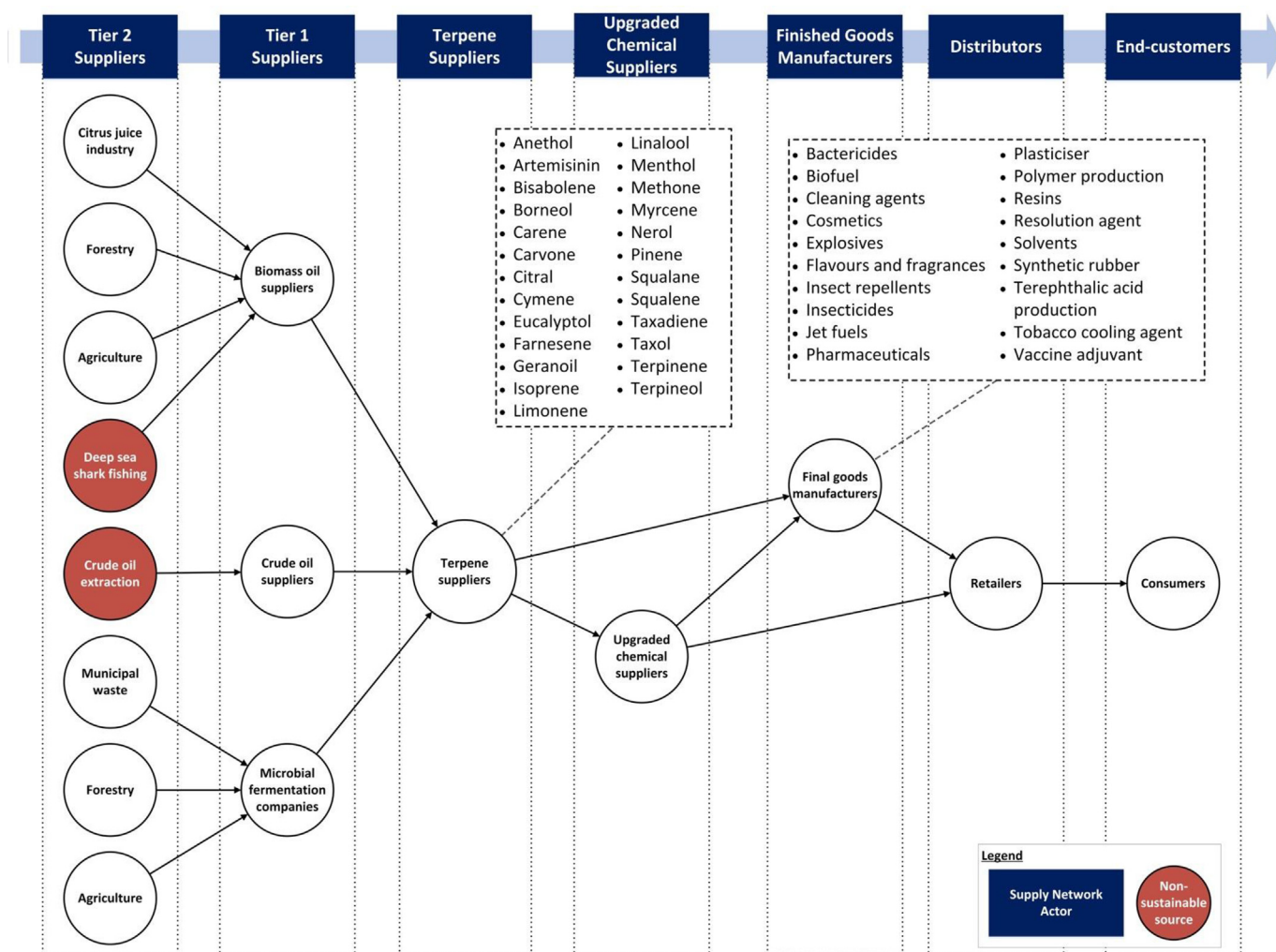


Fig. 6. Structure of supply networks defined by terpenoid renewable chemical feedstocks.

shapes 'market pull' phenomena by establishing the technological link between renewable feedstocks and commercial chemical-based products.

Considering that the primary processing of terpenoid feedstocks results in compounds with molecular impurities, specialty chemicals and catalytic transformations are required to ensure sustainable production, from a life cycle perspective, and upgrade the primary-derived terpenes to higher value raw materials. Increasing the purity of terpenes might be essential in complying with high quality standards for intermediates or end-products, like for the case of active pharmaceutical ingredients, as imposed by institutional actors and consumers. In this sense, combining innovative chemistry and process intensification are necessary to develop sustainable catalytic conversion routes of terpenes to replace expensive reagents, strong oxidants and environmentally polluting solvents.

Finished goods manufacturers can then incorporate the upgraded terpenes into their processes for engineering value-added functional products with market potential. The distribution of terpene-based offerings should stress the sustainable utilisation of renewable terpenoid feedstocks to align with the growing consumers' demand for non-petrochemical based products and contribute to the gradual decrease in the reliance upon fossil-based resources. End-consumers should be aware of the sustainable nature of the novel products and about any associated functional

benefits that could enhance market value.

Tracking the flow of terpenes across the SC might be challenging owing to the variety of natural and industrial sources of terpenoid feedstocks. Nonetheless, the depicted tier structure in Fig. 6 enables the understanding of network echelons in which the different actors and raw material sources are located, along with the associated capacity volumes (e.g. the citrus industry has a large footprint in Brazil and the United States of America – Florida and California). The geographical determination of terpenoid feedstocks can enable a structured analysis of supply and demand at each network tier.

Even though the analysis of network configuration, actors, and cost structure, might be readily attainable at the sources' network echelon, this becomes more challenging at the end-consumers' level due to the increasing complexity of the value chain structure. The complexity increases due to the multitude of possible processing routes and alternative products in the downstream supply network. Furthermore, ambiguities in the cost structure related to the SC are prevalent as many aspects thereof are still emerging and often confounded by the different by-products deriving during catalytic flow syntheses.

4.2. Uncertainty dimensions

Our engagement with the literature and the expert informants revealed five key dimensions of uncertainty regarding the case of

Table 7
Uncertainty dimensions impacting the value and viability of terpene-based circular supply networks.

Uncertainty dimension	Cause(s) of uncertainty
1. Omissions of feedstock sources, terpenes, processing routes and intermediates or end-products	<ul style="list-style-type: none"> • Fragmented nature of literature • Emerging and dynamic state of industry
2. Environmental and financial information	<ul style="list-style-type: none"> • Emerging and dynamic state of industry • Lack of information in academic domain
3. Product and market linkages	<ul style="list-style-type: none"> • Confounded data due to by-product nature • Emerging and dynamic state of industry • Lack of information in academic domain
4. Chemical synthesis and processing steps	<ul style="list-style-type: none"> • Complexity at the market side of supply network • Emerging and dynamic state of industry • Lack of information in academic/research domain
5. Future supply network governance and relationships	<ul style="list-style-type: none"> • Emerging and dynamic state of industry • Lack of information in academic domain

terpene-based circular supply networks. Each of the identified uncertainty dimensions can be linked to specific causes, as illustrated in Table 7.

5. Real-word paradigm: terpenoid feedstocks in pharmaceutical supply networks

Pharmaceutical companies tend to adopt a 'benign by design' approach to reduce environmental impact (Leder et al., 2015) while contemporarily retaining or even improving the pharmacological properties of medicines (Kümmerer and Hempel, 2010). To this effect, the environmental performance of national healthcare systems could be improved considering that these comprise the major clientele of pharmaceutical manufacturers (Ryan-Fogarty et al., 2016). Indicatively, the carbon footprint of England's National Healthcare System (NHS) is estimated to be 22.8 Mt CO₂-eq., 6.5% of which is attributed to the procurement of medical supplies (Sustainable Development Unit, 2016). However, the development of pharmaceutical SC theory and practice based on renewable chemical feedstocks is hindered by: (i) the reliance of the industry on vertically integrated petrochemical feedstock supply systems (Lamers et al., 2015); and (ii) the lack of research upon the technical feasibility of using renewable chemical feedstocks for manufacturing medications (Behr and Johnen, 2009).

An indicative example of using terpenoid feedstocks for the synthesis of 'green' pharmaceuticals (i.e. pharmaceuticals manufactured from renewable materials) is the case of paracetamol. Paracetamol, also known as acetaminophen and by its chemical name as N-(4-hydroxyphenyl)acetamide, is an active pharmaceutical ingredient which is widely used to manufacture non-steroidal analgesic medicines. In England, paracetamol is among the most prescribed medicines by the NHS, contributing circa 21% by quantity of active pharmaceutical ingredient (Penny and Collins, 2014). The selection of paracetamol as an exemplar case owes to the premise of our collaboration with leading European Chemicals SC businesses and academic stakeholders in the context of the acknowledged research projects. A research strand focuses on demonstrating, on a pilot scale, the terpene-based manufacturing process for 'green' paracetamol to showcase the advantages of terpenes as sustainable production inputs. Especially, chemical synthesis platforms for the conversion of β -pinene or limonene into 'green' paracetamol have been determined as very cost-effective and suitable for commercial applications (Lapkin et al., 2017).

Nowadays, over 300 pathways are reported for the chemical synthesis of paracetamol with the most commercially viable relying upon fossil-based feedstocks derived from benzene (Settanni et al., 2016), i.e. phenol, nitrobenzene and p-nitrochlorobenzene. In this regard, the global paracetamol market is economically supplied by chemical industries located in emerging

economies, mainly India and China. However, the exploitation of terpenes as renewable chemical feedstock sources highlights the possibility of different (re)configuration scenarios for the respective supply networks.

For example, considering that a sustainable viable source for β -pinene is paper and pulp industry waste, a possible scenario could assume that primary manufacturing operations for 'green' paracetamol are located close to paper and pulp mills, thus suggesting the reshoring of pharmaceutical primary manufacturing operations from emerging economies to Scandinavian countries. According to statistics provided by the Confederation of European Paper Industries, Scandinavian countries dominate the European pulp and paper production industry (CEPI, 2018). An alternative scenario could consider the use of citrus waste as a viable source of highly concentrated limonene for the synthesis of 'green' paracetamol, thus contributing to the reconfiguration of primary pharmaceutical manufacturing operations from India and China to Florida, United States of America, and Sao Paulo, Brazil, which are the leading regions in terms of global orange juice production (Gao et al., 2019).

A graphical illustration of a typical pharmaceutical supply system is depicted in Fig. 7, further indicating alternative SC configuration opportunities arising from renewable chemical feedstock platform technologies. The network structure does not extend to the research and development phases of biopharmaceuticals but focuses on pharmaceutical industrial systems' (re)configuration opportunities stemming from renewable chemical feedstocks. This representation is used to further inform our on-going, more targeted, research in modelling and quantifying the economic viability and environmental repercussions of terpenes in end-to-end pharmaceutical supply networks. In this regard, Tsolakis and Srai (2018) provide a systems-level mapping framework capturing the macro-level supply network dynamics governing 'green' pharmaceutical industrial networks enabled by renewable feedstocks.

6. Conclusions

This study contributes to sustainable SC research by investigating supply network designs defined by renewable chemical feedstock sources such as terpenes. In particular, the study adapts existing material-processing-supply network analysis techniques to the domain of compound class defined SCs and lays the foundations for quantitative environmental, economic and social modelling of renewable chemical feedstock-based networks. From a circular economy perspective, the developed network structure of SCs defined by terpenoid renewable chemical feedstocks and the presented case of 'green' paracetamol demonstrate the utility of the approach by integrating supply side considerations (i.e. feedstock) with uncertainties about intermediate processing options and commercialisation routes. The novelty of our approach is

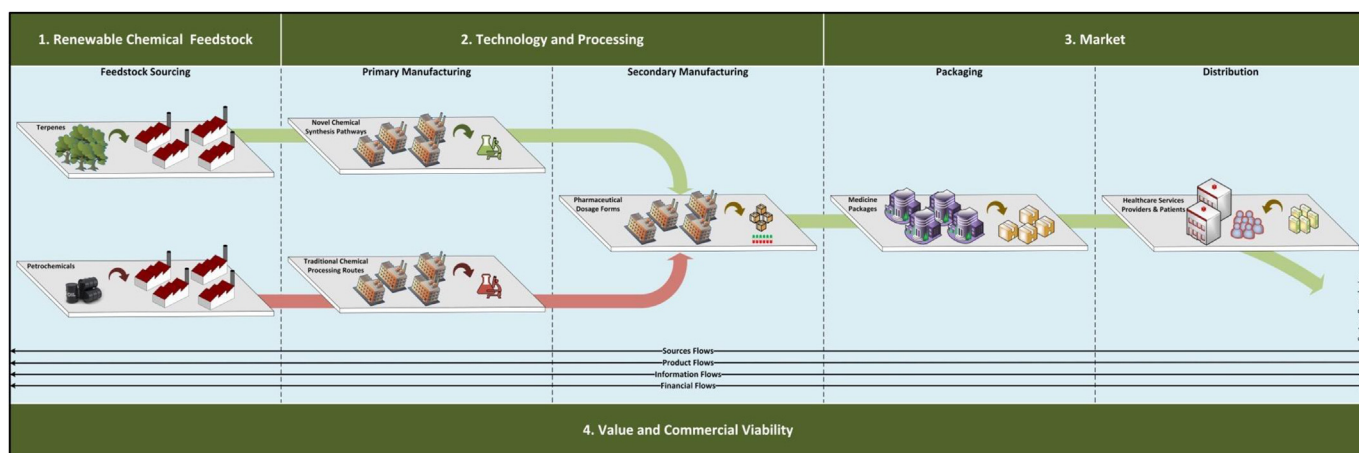


Fig. 7. Circular supply networks' structure and (re)configuration opportunities stemming from the exploitation of renewable chemical feedstock sources [Adapted from: Tsolakis and Srai (2018)].

encapsulated in the possible usefulness and challenges related to the application of the resulting compound class defined SC analysis techniques through providing a consolidated overview of the terpene industry and literature.

6.1. Key findings

The role of SC considerations (Martínez-Jurado and Moyano-Fuentes, 2014) and corporate strategy (Lozano et al., 2015) are documented as relevant towards enhancing firms' sustainability and crafting global value chains of the future. In this sense, this research considered the analysis of terpene-based renewable feedstock SC configurations. The case of terpenes was selected primarily due to the broad range of compounds that render them suitable for extending current knowledge regarding circular SCs defined by renewable chemical feedstocks (Eisenhardt and Graebner, 2007). A considerable number of publications addressing terpenes exists; however, the extant literature includes many articles that either discuss terpenes within the broader scope of addressing renewables (Zakzeski et al., 2010) or focus on natural processes involving terpenes without being relevant to their industrial extraction or commercial use (Zhang et al., 2014). To the best of our knowledge, there are not any studies that systematically investigate terpenes from a SC perspective. In this regard, we collated the dispersed literature on terpenoid feedstocks and demonstrate the diversity that exists within the family of terpenes. The present study further illustrates the broad range of sources, technology and processes, and commercial applications of terpenes that facilitate the positioning of terpene-based compounds in the SC field. Contemporarily, this research highlights novel (re)configuration opportunities for emerging bio-based industrial systems, thus helping to address Research Question #1. In particular, we describe the pharmaceutical SC potential of using either β -pinene or limonene as terpenoid feedstocks for the synthesis of 'green' paracetamol.

Furthermore, collating the dispersed literature on renewable chemical feedstocks in tandem with semi-structured interviews and expert panel engagements, involving industry and academic informants, are used to guide the design of SC operations defined by terpenoid feedstocks and tackle Research Question #2. The 'green' paracetamol case is used to demonstrate the real-world ramifications of terpenes on common products. In an attempt to answer Research Question #3, we identify key uncertainty dimensions and causes thereof regarding the design of circular

supply networks defined by terpenes, particularly referring to: environmental impact of end-to-end SC operations; feedstock supply and product demand patterns; chemical conversion pathways; financial considerations; and network governance and relationships.

6.1.1. Value chain analysis perspective

Based on emerging research aiming to enable the analysis of renewable chemical feedstock driven SCs in the context of uncertainty, this research presents a supply network design and analysis framework to investigate the financial and environmental value and viability of compound class defined networks. In particular, four fundamental theme areas are identified for investigation, namely: (i) renewable chemical feedstock sources; (ii) alternative technology and processing options; (iii) intermediate or end-user markets; and (iv) commercial value and viability. SC analysis based on these four theme areas allows for the structured identification of attractive value propositions that emerge from potential intermediate compounds derived from given feedstocks.

6.1.2. Structural implications

There has been significant research and commercial interest in exploring renewable chemical feedstocks to provide alternatives to petrochemical sources. However, unlike customer demand-driven supply chains (SCs) where there are established methodologies for identifying target markets, products and production processes, the exploration of alternative renewable feedstocks requires network structural considerations from a raw material perspective. Thereafter, the order of processing options and conversion pathways for the elaborated renewable chemical feedstocks requires structured mapping of the emerging SCs as the variety of possible commercial products increases in the downstream operations. Compound class defined material-processing-supply network structures are then determined based on business value and viability targets. In addition, inventory planning and control of renewable feedstocks is a critical constituent that dictates the configurational structure of the emerging circular supply networks (Tsolakis and Srai, 2017).

6.1.3. Uncertainties' accountability

Previous research has suggested that utilising renewable chemical feedstocks may be considered a strategic advantage for a plethora of industrial sectors (Okoro et al., 2017) and an opportunity to foster the transition to a circular economy era (Tsolakis et al.,

2016). However, this transition requires significant changes in SC design and analysis techniques. In particular, techniques are needed that can support network design in the face of multiple uncertainties, including feedstock availability and quality, new or emerging process pathways and technologies, and a complex set of intermediate or end-use markets. This stands in contrast to conventional SC design and analysis where incremental improvements are often sought in established end-to-end systems or where the solution space can be more narrowly defined by specific markets, technologies or products. This enables much better certainty regarding key variables in the SC that underpin viability. The described case study about 'green' paracetamol not only presents important findings regarding the uncertainties that need to be addressed to enable the successful introduction of terpene-based chemical SCs, but also highlights several challenges facing the introduction of renewable chemical feedstocks in general.

6.2. Limitations

This study has inherent limitations. Constructing the mapping approach requires the collation of data from a variety of sources and it was not possible to represent data that was not fully understood in context. In addition, the proposed mapping approach may not be sufficient to capture the complexity, economic and environmental aspects of the processing routes in a compound class defined supply network. Furthermore, the provision of a detailed map with possible market volumes might require extensive data collection from a variety of sources. Most noticeably, the study fails to account for the interaction between feedstock volumes and prices and the market acceptability of the derived commercial offerings. Moreover, our study considers renewable material flows; however, to better inform chemical process and product designs a pallet of considerations is necessitated (Machado et al., 2018), including: energy flows and efficiency; carbon dioxide emissions; and toxic and bio-accumulative substances' generation.

6.3. Future research

Future research on the value and viability of renewable chemical feedstocks could address the detailed causes of uncertainty to result in a more industry-focused approach to gain information that

is not available in academic publications (Mitsos et al., 2018). Research that collates findings at a higher level of analysis, as presented here, is key to better analysing the viability of renewable chemical feedstock solutions. In this sense, it will be necessary to use methods that can evaluate the relevant economics within the confounded by-product environment in which they are often produced (Gold and Seuring, 2011). Furthermore, a more market-driven approach could provide a focused scope that enables a better linkage among feedstock sources, compound-based intermediates and end-products (Homrich et al., 2018). Finally, additional research could expand this study by investigating other cases of renewable chemical feedstocks to ensure generalisability (Ko et al., 2018), while further improving the proposed framework through more extensive testing.

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Appendix

Table A1
Informants' expertise and key insights.

Sector/Field	Specific Expertise	Interview Main Points and Insights
Chemistry	Chemical routes to process terpenes, as part of an EPSRC funded project Organic chemistry synthesis routes	<ul style="list-style-type: none"> Chemical processing of terpenes into value-added products is a key area of focus for research and industry actors. Polymer categories (e.g. monomers to produce PET), could be partially produced from terpenes. Chemical synthesis pathways to produce polymers still need to be developed in a viable manner. Polymer market presents opportunities to replace petrochemical feedstocks. Polymers manufactured from renewable chemical feedstocks could be different from traditional petrochemical-based plastics. 'Green' polymers should be produced, and their properties need to be tested experimentally. Fragrances and flavours appear to be the primary market that drives the developments in the field of renewable chemical feedstocks for value-added chemicals. Research currently focuses on intensifying processing of renewable chemical to enable industrial scale production and commercialisation. Alternative chemical synthesis pathways are experimentally explored to derive the same intermediate or end-product, with the associated barriers and challenges being investigated. Reaction kinetics and technical process models of terpenes are within the focus of chemical engineers.
	Inorganic chemistry synthesis routes, as part of an EPSRC funded project	
Biology and biochemistry	Microbial fermentation routes to terpenes	
Chemical engineering	Process intensification of terpene reactions	
	Sustainable reaction engineering, chemical engineering and biotechnology	

Table A1 (continued)

Sector/Field	Specific Expertise	Interview Main Points and Insights
	Epoxidation of limonene (a specific terpenoid feedstock)	<ul style="list-style-type: none"> Chemical engineers explore data sets for the reliable technical assessment of terpenes as viable a renewable chemical feedstock. Mapping the details of renewable chemical feedstock related reactions is non-trivial. Lack of adequate experimental data over the chemical processing models is crucial to document the related reactions.
	Chemical processes' intensification	<ul style="list-style-type: none"> Commercially viable renewable chemical feedstocks need to be supported by research evidence and market demand opportunities.
Systems engineering	Analysis, design and operation of international production, supply and service networks Design of nascent networks for emerging technologies/industries	<ul style="list-style-type: none"> Supply chains arising from renewable chemical feedstocks require a holistic determination of viability. Replacing petrochemical compounds with natural feedstocks is still costly, hence hindering the synthetic production of value-added intermediates or end-products.
Renewable chemical feedstocks	Integrated supply and processing pipeline for the sustained production of fuels, as part of an ESPRC funded project Ionic liquid biorefining of lignocellulose to sustainable polymers, as part of an ESPRC funded project	<ul style="list-style-type: none"> Energy balance calculations are necessary to determine the benefits of energy solutions stemming from renewable chemical feedstocks. Biomass can be broken down into cellulose, hemi-cellulose and lignin. Lignin tends to vary considerably between different plants/species and even parts of the same plant. Bio-refineries need to be able to process a wide spectrum of biomass types in order to be viable.
	Bio-derived feedstocks for sustainable, UK-based manufacture of chemicals and pharmaceutical intermediates, as part of an ESPRC funded project	<ul style="list-style-type: none"> Pharmaceutical companies are willing to replace petrochemical feedstocks with renewable counterparts owing to oil variable price and the expected market competitive advantage due to branding a 'green' image.
Pharmaceuticals	Development, supply and service for diagnostics	<ul style="list-style-type: none"> Potential renewable chemical feedstocks to manufacture pharmaceuticals should be evaluated through multi-utility attribute or multivariable analytical techniques. Significant fossil feedstocks for pharmaceuticals are: Salicylic acid, Ethylene glycol, Acrylonitrile, Formaldehyde, and Acetic acid.

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